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Towrards a Chemistry and Molecular & Materials Science Virtual Research Community

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Impact

Two levels of impact (the VO and the Infrastructure) on the whole computing framework having distinctive characteristics have been operated. In particular:
a) at the VO level: two main skeletons, planned as case studies, have been developed to tackle the problem of properly distributing HTC and HPC components on the most suited platform will be de-signed;
b) at the Infrastructure level: access to different HPC computing platforms and storing resources have been enabled at a (unified) middleware level to interoperate to the end of optimally handling a given application.
Another important impact has been that of separating users in layers and more than production quantity the corresponding quality is rewarded

URL

http://www.chm.unipg.it/

Summary

To foster the development of the Chemistry and Molecular and Materials Science and Technology (CMMST) community within EGI, a frame-work called GriF has been developed. Leveraging on the fact that the largest number of CMMST researchers gathered within EGI are aggregated around the COMPCHEM VO and work at the assemblage and development of the components of GEMS (the Grid Empowered Molecular Simulator) our activity has focused on making GriF (a Grid framework) facilitate the assemblage of the various packages in a suitable workflow and foster interoperability between HPC and HPC platforms. In doing this GriF, that has been structured in a way that allows the collection of information useful to evaluate quality of services and of the users is used as a means to boost the growth of the CMMST community.

Description

The participation of the Chemistry and Molecular and Materials Science and Technology (CMMST) community to EGI is rather fragmented or ancillary to other scientific fields. The largest number of CMMST researchers has been aggregated around the COMPCHEM VO whose key activity is to assemble components of GEMS [1] (the Grid Empowered Molecular Simulator). The assemblage of GEMS components is based on the implementation of various CMMST packages whose computer demand is highly variable depending on the scale of the treatment and the accuracy required. To foster the growth of the CMMST community a grid framework called GriF [2,3] has been developed that facilitates the assemblage of such packages and allows interoperability between HPC and HPC plat-forms (in the work performed interoperation was achieved between the section of the IGI (Italian Grid Infrastructure) Grid and the HPC platform of CINECA (the largest supercomputer platform in Italy) using a WMS-driven bridge over the SSH protocol. GriF allows at the same time the assemblage of a proper workflow and a quality evaluation of the services (and of the users as well) that has shown to be vital for the establishing of collaboration among the CMMST researchers members of COMP-CHEM [4].
The following general steps had to be undertaken:
- identify the HPC platforms willing to support the project by opening the use of their resources allo-cated to the Grid,
- allow the users access the involved platforms,
- identify a middleware solution suited to operate both on HPC platforms and the EGI Grid,

- integrate HPC/HTC workflows by adapting the GriF server for communicating with the new mid-dleware layer,
- transform the application(s) into (HPC/HTC) workflows and adapt the GriF client for running,
- adapt the GriF database for improving the quality system.

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